

Acetic acid

64-19-7 | DTXSID5024394

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $8.20\text{e-}13 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $4.87\text{e-}01$

Confidence level: $7.16\text{e-}01$

Nearest Neighbors from the Training Set

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Acetic acid

Measured: $7.40\text{e-}13$

Predicted: $8.20\text{e-}13$

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Propionic acid

Measured: $1.22\text{e-}12$

Predicted: $1.27\text{e-}12$

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Methyl acetate

Measured: $3.41\text{e-}13$

Predicted: $6.02\text{e-}13$

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2-Methylpropanoic acid

Measured: $2.00\text{e-}12$

Predicted: $1.95\text{e-}12$

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Methyl 2-hydroxypropanoate

Measured: $2.80\text{e-}12$

Predicted: $3.16\text{e-}12$